Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2023 – 10:39 PM EDT

PDB ID	:	3CYU
Title	:	Human Carbonic Anhydrase II complexed with Cryptophane biosensor and xenon
Authors	:	Aaron, J.A.; Jude, K.M.; Di Costanzo, L.; Christianson, D.W.
Deposited on	:	2008-04-26
Resolution	:	1.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

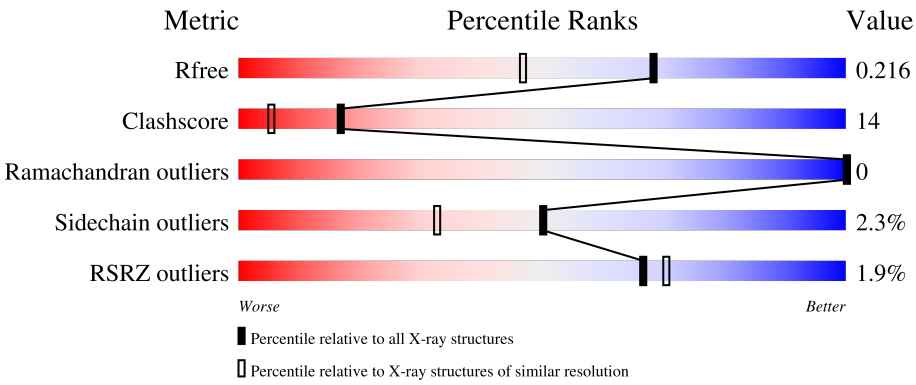
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	260	2% 79% 18% ··

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	0CR	A	263[A]	-	X	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	1CR	A	264[B]	-	X	-	X
5	XE	A	266	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 2443 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

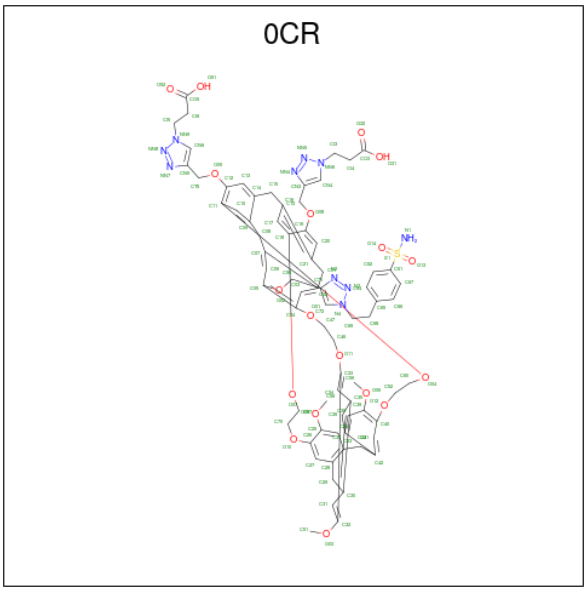
- Molecule 1 is a protein called Carbonic anhydrase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	257	2049	1315	352	380	2	0	0	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

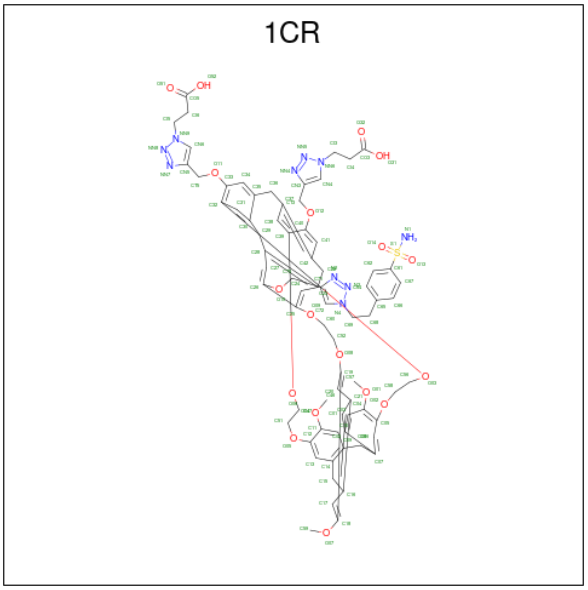
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	1	1	1	0	0

- Molecule 3 is MoMo-2-[4-(2-(4-(methoxy)-1H-1,2,3-triazol-1-yl)ethyl)benzenesulfonamide]-7,12-bis-[3-(4-(methoxy)-1H-1,2,3-triazol-1-y l)propanoic acid]-cryptophane-A (three-letter code: 0CR) (formula: $C_{74}H_{74}N_{10}O_{18}S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	103	74	10	18	1	0	1

- Molecule 4 is PoPo-2-[4-(2-(4-(methoxy)-1H-1,2,3-triazol-1-yl)ethyl)benzenesulfonamide]-7,12-bis-[3-(4-(methoxy)-1H-1,2,3-triazol-1-yl)propanoic acid]-cryptophane-A (three-letter code: 1CR) (formula: $C_{74}H_{74}N_{10}O_{18}S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	A	1	103	74	10	18	1	0	1

- Molecule 5 is XENON (three-letter code: XE) (formula: Xe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Xe		
5	A	2	2	2	0	0

- Molecule 6 is water.

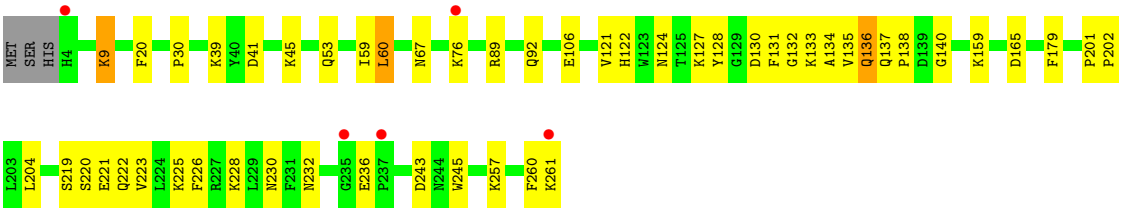
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	185	185	185	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Carbonic anhydrase 2

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	67.44Å 49.98Å 81.04Å 90.00° 107.13° 90.00°	Depositor
Resolution (Å)	38.72 – 1.70 39.50 – 1.70	Depositor EDS
% Data completeness (in resolution range)	90.6 (38.72-1.70) 90.4 (39.50-1.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.84 (at 1.70Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.226 , 0.249 0.216 , 0.216	Depositor DCC
R_{free} test set	1139 reflections (4.11%)	wwPDB-VP
Wilson B-factor (Å^2)	20.9	Xtriage
Anisotropy	0.952	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 57.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	2443	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.20% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: XE, 0CR, ZN, 1CR

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.34	0/2110	0.63	0/2862

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2049	0	2002	59	0
2	A	1	0	0	0	0
3	A	103	0	68	4	0
4	A	103	0	72	7	0
5	A	2	0	0	3	0
6	A	185	0	0	0	0
All	All	2443	0	2142	62	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (62) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:264[B]:1CR:NN6	4:A:264[B]:1CR:CI3	1.68	1.54
4:A:264[B]:1CR:CI3	4:A:264[B]:1CR:CN4	2.48	0.92
1:A:128:TYR:CZ	1:A:137:GLN:HG2	2.18	0.79
1:A:128:TYR:OH	1:A:137:GLN:HG2	1.86	0.76
1:A:128:TYR:O	1:A:133:LYS:HD2	1.85	0.75
1:A:226:PHE:CD2	5:A:266:XE:XE	3.19	0.74
1:A:131:PHE:O	1:A:135:VAL:HG23	1.89	0.72
1:A:261:LYS:N	1:A:261:LYS:HE2	2.12	0.65
1:A:39:LYS:HB2	1:A:39:LYS:NZ	2.14	0.61
1:A:9:LYS:N	1:A:9:LYS:HD3	2.16	0.61
1:A:130:ASP:OD2	1:A:133:LYS:HG3	2.02	0.60
1:A:223:VAL:HG23	5:A:266:XE:XE	2.81	0.59
1:A:130:ASP:CG	1:A:133:LYS:HE2	2.24	0.58
1:A:9:LYS:H	1:A:9:LYS:CD	2.16	0.57
1:A:39:LYS:HB2	1:A:39:LYS:HZ3	1.68	0.57
1:A:128:TYR:HH	1:A:137:GLN:HG2	1.69	0.56
1:A:132:GLY:HA3	4:A:264[B]:1CR:H59	1.87	0.56
1:A:135:VAL:HG12	1:A:204:LEU:HD12	1.87	0.56
1:A:121:VAL:HG21	4:A:264[B]:1CR:H67	1.90	0.53
1:A:121:VAL:HG21	3:A:263[A]:0CR:H67	1.90	0.53
1:A:260:PHE:HD2	1:A:261:LYS:HE3	1.73	0.53
1:A:232:ASN:HB2	1:A:236:GLU:HG3	1.91	0.52
1:A:9:LYS:HD3	1:A:9:LYS:H	1.75	0.52
1:A:226:PHE:CE2	5:A:266:XE:XE	3.41	0.51
4:A:264[B]:1CR:CN4	4:A:264[B]:1CR:HI3	2.38	0.51
1:A:137:GLN:HG3	1:A:138:PRO:HD2	1.93	0.51
1:A:45:LYS:HE2	1:A:45:LYS:H	1.75	0.50
1:A:124:ASN:OD1	1:A:127:LYS:HG2	2.11	0.50
1:A:136:GLN:NE2	4:A:264[B]:1CR:C41	2.75	0.48
1:A:9:LYS:N	1:A:9:LYS:CD	2.76	0.48
1:A:89:ARG:O	1:A:122:HIS:HA	2.14	0.48
1:A:202:PRO:HG3	3:A:263[A]:0CR:H46	1.96	0.48
1:A:221:GLU:O	1:A:225:LYS:HG2	2.15	0.47
1:A:39:LYS:NZ	1:A:39:LYS:CB	2.76	0.47
1:A:45:LYS:N	1:A:45:LYS:HD3	2.30	0.46
1:A:220:SER:HA	1:A:223:VAL:HG12	1.98	0.46
1:A:60:LEU:C	1:A:60:LEU:HD22	2.37	0.46
1:A:20:PHE:CE2	1:A:201:PRO:HB3	2.52	0.45
1:A:260:PHE:HB2	1:A:261:LYS:HE2	2.00	0.44
1:A:53:GLN:HB2	1:A:76:LYS:O	2.18	0.44
1:A:230:ASN:HB3	1:A:232:ASN:OD1	2.18	0.44
1:A:260:PHE:HB2	1:A:261:LYS:CE	2.47	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:LEU:HD13	1:A:60:LEU:N	2.33	0.43
1:A:219:SER:OG	1:A:222:GLN:HG3	2.19	0.43
1:A:260:PHE:CD2	1:A:261:LYS:HG2	2.54	0.43
1:A:159:LYS:HD3	1:A:179:PHE:HD1	1.83	0.42
1:A:243:ASP:HA	1:A:245:TRP:CD1	2.54	0.42
1:A:228:LYS:CB	1:A:228:LYS:NZ	2.83	0.42
1:A:53:GLN:O	1:A:76:LYS:HB2	2.19	0.42
1:A:220:SER:O	1:A:223:VAL:HG12	2.20	0.42
1:A:202:PRO:HG3	3:A:263[A]:0CR:C46	2.49	0.41
1:A:59:ILE:HA	1:A:67:ASN:O	2.19	0.41
1:A:124:ASN:CG	1:A:127:LYS:HG2	2.41	0.41
1:A:260:PHE:O	1:A:261:LYS:HB2	2.21	0.41
1:A:60:LEU:HD13	1:A:60:LEU:H	1.85	0.41
1:A:41:ASP:OD1	1:A:257:LYS:HD3	2.21	0.41
1:A:202:PRO:HD3	4:A:264[B]:1CR:H70	2.03	0.41
1:A:30:PRO:HG3	1:A:106:GLU:HB3	2.03	0.40
1:A:134:ALA:O	1:A:140:GLY:HA3	2.22	0.40
1:A:131:PHE:CE1	1:A:135:VAL:HG21	2.56	0.40
1:A:136:GLN:NE2	3:A:263[A]:0CR:C20	2.85	0.40
1:A:135:VAL:CG1	1:A:204:LEU:HD12	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	255/260 (98%)	243 (95%)	12 (5%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	222/225 (99%)	217 (98%)	5 (2%)	50 33

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	60	LEU
1	A	92	GLN
1	A	136	GLN
1	A	165	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	136	GLN
1	A	137	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| >$
3	0CR	A	263[A]	2	116,116,116	3.16	64 (55%)	154,166,166	3.27	59 (38%
4	1CR	A	264[B]	2	116,116,116	2.97	65 (56%)	154,166,166	3.65	59 (38%

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	0CR	A	263[A]	2	-	48/81/87/87	0/4/14/14
4	1CR	A	264[B]	2	-	42/81/87/87	0/4/14/14

All (129) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	264[B]	1CR	CI3-NN6	12.19	1.68	1.47
3	A	263[A]	0CR	CT5-CN5	-8.70	1.28	1.50
3	A	263[A]	0CR	O01-C04	7.99	1.53	1.37
3	A	263[A]	0CR	O06-C39	7.90	1.49	1.37
3	A	263[A]	0CR	O02-C05	7.73	1.52	1.37
3	A	263[A]	0CR	O08-C19	7.67	1.52	1.37
3	A	263[A]	0CR	O05-C12	7.56	1.52	1.37
4	A	264[B]	1CR	O01-C04	7.35	1.48	1.37
3	A	263[A]	0CR	O04-C11	6.96	1.51	1.37
3	A	263[A]	0CR	CT3-CN3	-6.79	1.33	1.50
3	A	263[A]	0CR	CI3-NN6	-6.28	1.37	1.47
4	A	264[B]	1CR	O04-C11	6.21	1.47	1.37
3	A	263[A]	0CR	O10-C26	6.15	1.49	1.37
3	A	263[A]	0CR	O07-C18	6.08	1.49	1.37
4	A	264[B]	1CR	O06-C39	6.07	1.49	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	264[B]	1CR	O02-C05	5.93	1.49	1.37
3	A	263[A]	0CR	O03-C32	5.85	1.46	1.37
3	A	263[A]	0CR	CI3-CI4	-5.85	1.30	1.51
4	A	264[B]	1CR	O01-C57	5.84	1.60	1.42
4	A	264[B]	1CR	C72-N4	-5.74	1.29	1.35
4	A	264[B]	1CR	O10-C70	-5.47	1.25	1.43
4	A	264[B]	1CR	O10-C26	5.26	1.48	1.37
4	A	264[B]	1CR	CN4-NN6	5.23	1.40	1.35
4	A	264[B]	1CR	O08-C19	5.02	1.47	1.37
4	A	264[B]	1CR	C71-N2	4.91	1.40	1.34
3	A	263[A]	0CR	O11-C33	4.86	1.47	1.37
3	A	263[A]	0CR	O14-S1	4.80	1.52	1.43
4	A	264[B]	1CR	O14-S1	4.80	1.52	1.43
4	A	264[B]	1CR	O11-C33	4.58	1.46	1.37
4	A	264[B]	1CR	CT3-CN3	4.57	1.61	1.50
3	A	263[A]	0CR	C71-N2	4.18	1.39	1.34
4	A	264[B]	1CR	O05-C12	4.13	1.45	1.37
4	A	264[B]	1CR	C70-C71	-4.00	1.40	1.50
4	A	264[B]	1CR	NN8-NN9	4.00	1.42	1.34
3	A	263[A]	0CR	O09-C25	3.92	1.43	1.37
3	A	263[A]	0CR	CN5-NN7	3.88	1.39	1.34
4	A	264[B]	1CR	O32-CO3	3.58	1.34	1.22
3	A	263[A]	0CR	O13-S1	3.56	1.50	1.43
4	A	264[B]	1CR	O13-S1	3.56	1.50	1.43
3	A	263[A]	0CR	C72-N4	-3.54	1.31	1.35
4	A	264[B]	1CR	O03-C32	3.48	1.44	1.37
4	A	264[B]	1CR	CN3-NN4	3.39	1.38	1.34
4	A	264[B]	1CR	C03-C04	3.38	1.44	1.38
3	A	263[A]	0CR	O52-CO5	3.29	1.33	1.22
3	A	263[A]	0CR	CN4-CN3	3.28	1.41	1.36
4	A	264[B]	1CR	O07-C18	3.27	1.42	1.37
3	A	263[A]	0CR	O05-CT5	-3.25	1.32	1.43
3	A	263[A]	0CR	CN3-NN4	3.23	1.38	1.34
4	A	264[B]	1CR	CN6-CN5	3.22	1.41	1.36
3	A	263[A]	0CR	NN8-NN9	3.12	1.40	1.34
3	A	263[A]	0CR	NN4-NN5	-3.12	1.28	1.34
4	A	264[B]	1CR	CI5-CI6	3.04	1.62	1.51
3	A	263[A]	0CR	O06-C59	3.04	1.51	1.42
3	A	263[A]	0CR	C27-C28	3.03	1.44	1.39
3	A	263[A]	0CR	CN4-NN6	3.01	1.38	1.35
4	A	264[B]	1CR	O03-C56	-2.95	1.33	1.43
3	A	263[A]	0CR	C58-C71	-2.91	1.43	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	264[B]	1CR	C34-C35	2.91	1.44	1.39
3	A	263[A]	0CR	C62-C61	2.89	1.43	1.38
4	A	264[B]	1CR	C62-C61	2.89	1.43	1.38
4	A	264[B]	1CR	C69-N4	-2.88	1.42	1.47
3	A	263[A]	0CR	C38-C37	2.82	1.44	1.39
3	A	263[A]	0CR	C03-C04	2.81	1.43	1.38
4	A	264[B]	1CR	C27-C28	2.80	1.44	1.39
4	A	264[B]	1CR	C20-C19	2.78	1.43	1.38
3	A	263[A]	0CR	O32-CO3	2.76	1.31	1.22
3	A	263[A]	0CR	C17-C18	2.72	1.43	1.38
3	A	263[A]	0CR	C27-C26	2.70	1.43	1.38
4	A	264[B]	1CR	C31-C30	2.65	1.44	1.39
3	A	263[A]	0CR	C34-C35	2.64	1.44	1.39
4	A	264[B]	1CR	C35-C30	2.63	1.45	1.40
3	A	263[A]	0CR	C64-C62	2.62	1.43	1.38
4	A	264[B]	1CR	C64-C62	2.62	1.43	1.38
3	A	263[A]	0CR	O11-C46	-2.60	1.34	1.43
3	A	263[A]	0CR	C10-C11	2.59	1.43	1.38
3	A	263[A]	0CR	C20-C21	2.58	1.43	1.39
3	A	263[A]	0CR	C35-C30	2.58	1.45	1.40
4	A	264[B]	1CR	CI6-CO5	2.58	1.56	1.50
4	A	264[B]	1CR	O04-C46	-2.57	1.35	1.42
3	A	263[A]	0CR	C34-C33	2.56	1.43	1.38
3	A	263[A]	0CR	C38-C39	2.55	1.43	1.38
4	A	264[B]	1CR	C20-C21	2.55	1.43	1.39
3	A	263[A]	0CR	C67-C61	2.52	1.42	1.38
4	A	264[B]	1CR	C67-C61	2.52	1.42	1.38
3	A	263[A]	0CR	O09-C56	2.52	1.50	1.42
3	A	263[A]	0CR	C06-C05	2.51	1.43	1.38
3	A	263[A]	0CR	S1-N1	2.50	1.65	1.60
4	A	264[B]	1CR	S1-N1	2.50	1.65	1.60
3	A	263[A]	0CR	CN6-CN5	2.49	1.39	1.36
4	A	264[B]	1CR	C10-C09	2.47	1.43	1.39
4	A	264[B]	1CR	C27-C26	2.47	1.43	1.38
3	A	263[A]	0CR	C70-C57	-2.47	1.36	1.49
3	A	263[A]	0CR	C13-C12	2.46	1.43	1.38
4	A	264[B]	1CR	CN5-NN7	2.45	1.37	1.34
4	A	264[B]	1CR	CN4-CN3	2.42	1.39	1.36
4	A	264[B]	1CR	C03-C02	2.41	1.43	1.39
3	A	263[A]	0CR	CI5-CI6	2.38	1.60	1.51
4	A	264[B]	1CR	C34-C33	2.36	1.43	1.38
4	A	264[B]	1CR	C13-C12	2.36	1.43	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	263[A]	0CR	C31-C30	2.32	1.43	1.39
4	A	264[B]	1CR	C21-C16	2.32	1.44	1.40
4	A	264[B]	1CR	C17-C16	2.31	1.43	1.39
4	A	264[B]	1CR	O09-C25	2.30	1.42	1.37
4	A	264[B]	1CR	C10-C11	2.29	1.43	1.38
4	A	264[B]	1CR	C38-C39	2.28	1.42	1.38
3	A	263[A]	0CR	C41-C42	2.27	1.43	1.39
4	A	264[B]	1CR	C13-C14	2.27	1.43	1.39
4	A	264[B]	1CR	CI3-CI4	-2.26	1.43	1.51
3	A	263[A]	0CR	C12-C11	2.23	1.45	1.40
3	A	263[A]	0CR	C42-C37	2.22	1.44	1.40
3	A	263[A]	0CR	C20-C19	2.21	1.42	1.38
3	A	263[A]	0CR	C64-C65	2.21	1.43	1.38
4	A	264[B]	1CR	C64-C65	2.21	1.43	1.38
4	A	264[B]	1CR	C38-C37	2.20	1.43	1.39
3	A	263[A]	0CR	C67-C66	2.14	1.42	1.38
4	A	264[B]	1CR	C67-C66	2.14	1.42	1.38
4	A	264[B]	1CR	C17-C18	2.13	1.42	1.38
4	A	264[B]	1CR	C14-C09	2.12	1.44	1.40
4	A	264[B]	1CR	C06-C05	2.10	1.42	1.38
3	A	263[A]	0CR	C14-C09	2.09	1.44	1.40
4	A	264[B]	1CR	O11-CT5	2.08	1.50	1.43
4	A	264[B]	1CR	C31-C32	2.05	1.42	1.38
3	A	263[A]	0CR	C41-C40	2.05	1.42	1.38
3	A	263[A]	0CR	C10-C09	2.04	1.43	1.39
4	A	264[B]	1CR	O12-CT3	2.04	1.50	1.43
3	A	263[A]	0CR	C60-C52	2.03	1.59	1.49
4	A	264[B]	1CR	C41-C42	2.02	1.43	1.39
4	A	264[B]	1CR	C41-C40	2.02	1.42	1.38
3	A	263[A]	0CR	C13-C14	2.02	1.43	1.39

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	264[B]	1CR	C70-O10-C26	18.87	154.90	117.76
4	A	264[B]	1CR	CT5-O11-C33	15.67	148.61	117.76
3	A	263[A]	0CR	O08-CT3-CN3	10.87	138.67	109.42
4	A	264[B]	1CR	O12-CT3-CN3	10.74	138.34	109.42
4	A	264[B]	1CR	CI3-NN6-CN4	-9.97	106.36	129.82
3	A	263[A]	0CR	CT3-CN3-CN4	-9.43	110.64	128.45
4	A	264[B]	1CR	O10-C70-C71	9.39	134.69	109.42
3	A	263[A]	0CR	O11-C46-C47	9.34	140.33	108.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	264[B]	1CR	CT3-O12-C40	9.20	135.87	117.76
4	A	264[B]	1CR	CI4-CI3-NN6	9.03	126.70	111.35
4	A	264[B]	1CR	CI6-CI5-NN9	8.50	125.79	111.35
3	A	263[A]	0CR	O51-CO5-O52	-8.40	102.36	123.30
3	A	263[A]	0CR	O51-CO5-CI6	8.37	140.93	114.03
3	A	263[A]	0CR	O14-S1-N1	8.19	119.51	107.36
4	A	264[B]	1CR	O14-S1-N1	8.19	119.51	107.36
3	A	263[A]	0CR	O01-C47-C46	8.17	136.38	108.72
4	A	264[B]	1CR	O07-C18-C19	8.16	126.78	115.41
4	A	264[B]	1CR	C57-O01-C04	-8.10	105.31	117.53
3	A	263[A]	0CR	O14-S1-O13	-7.77	105.99	118.76
4	A	264[B]	1CR	O14-S1-O13	-7.77	105.99	118.76
3	A	263[A]	0CR	O08-C19-C18	7.57	131.37	115.73
3	A	263[A]	0CR	C51-O03-C32	7.54	128.91	117.53
3	A	263[A]	0CR	O05-CT5-CN5	7.22	128.85	109.42
3	A	263[A]	0CR	O07-C18-C19	7.20	130.59	115.73
3	A	263[A]	0CR	O12-C52-C60	6.66	131.27	108.72
3	A	263[A]	0CR	NN4-NN5-NN6	6.37	112.12	107.31
3	A	263[A]	0CR	O04-C60-C52	5.81	128.37	108.72
3	A	263[A]	0CR	O07-C18-C17	-5.70	110.47	123.58
3	A	263[A]	0CR	O05-C12-C11	5.70	127.51	115.73
3	A	263[A]	0CR	C09-C08-C07	5.51	124.37	112.91
4	A	264[B]	1CR	O07-C18-C17	-5.30	114.99	124.12
4	A	264[B]	1CR	O52-CO5-O51	-5.24	110.24	123.30
3	A	263[A]	0CR	O08-C19-C20	-5.20	111.63	123.58
4	A	264[B]	1CR	O08-C19-C18	5.17	126.42	115.73
3	A	263[A]	0CR	C16-C15-C14	5.08	123.48	112.91
3	A	263[A]	0CR	CN4-CN3-NN4	-5.02	103.88	111.34
4	A	264[B]	1CR	NN4-NN5-NN6	4.65	110.82	107.31
4	A	264[B]	1CR	CN4-CN3-NN4	-4.62	104.48	111.34
4	A	264[B]	1CR	O11-CT5-CN5	4.60	121.81	109.42
3	A	263[A]	0CR	O05-C12-C13	-4.30	113.70	123.58
3	A	263[A]	0CR	O01-C04-C05	4.30	124.60	115.73
4	A	264[B]	1CR	CT3-CN3-CN4	-4.18	120.55	128.45
4	A	264[B]	1CR	C47-O06-C39	4.10	127.72	117.69
3	A	263[A]	0CR	CI6-CI5-NN9	4.02	118.18	111.35
3	A	263[A]	0CR	C68-C69-N4	3.98	118.12	111.35
3	A	263[A]	0CR	C15-C14-C09	3.88	128.99	123.56
3	A	263[A]	0CR	CT5-O05-C12	3.83	125.30	117.76
4	A	264[B]	1CR	C30-C29-C28	-3.81	104.99	112.91
3	A	263[A]	0CR	C72-C71-N2	-3.78	105.72	111.34
3	A	263[A]	0CR	C47-O01-C04	-3.69	108.66	117.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	263[A]	0CR	C30-C29-C28	-3.65	105.32	112.91
3	A	263[A]	0CR	C69-C68-C65	3.64	123.06	112.55
3	A	263[A]	0CR	C22-C42-C37	3.64	128.65	123.56
4	A	264[B]	1CR	O08-C19-C20	-3.57	115.37	123.58
4	A	264[B]	1CR	O05-C51-C47	3.49	120.54	108.72
4	A	264[B]	1CR	C42-C22-C23	3.47	120.12	112.91
4	A	264[B]	1CR	C52-O08-C19	-3.46	109.23	117.69
3	A	263[A]	0CR	C67-C61-S1	3.45	124.74	119.73
4	A	264[B]	1CR	C67-C61-S1	3.45	124.74	119.73
4	A	264[B]	1CR	O02-C05-C06	3.41	131.43	123.58
3	A	263[A]	0CR	C57-O07-C18	3.38	125.95	117.69
3	A	263[A]	0CR	C61-S1-N1	-3.34	103.66	108.38
4	A	264[B]	1CR	C61-S1-N1	-3.34	103.66	108.38
4	A	264[B]	1CR	O02-C05-C04	-3.34	108.83	115.73
4	A	264[B]	1CR	C69-N4-C72	-3.25	122.18	129.82
4	A	264[B]	1CR	C09-C08-C07	3.25	119.66	112.91
3	A	263[A]	0CR	CN6-CN5-NN7	-3.24	106.53	111.34
3	A	263[A]	0CR	NN7-NN8-NN9	-3.22	104.89	107.31
3	A	263[A]	0CR	C70-O10-C26	-3.19	109.88	117.69
4	A	264[B]	1CR	C72-C71-N2	-3.18	106.61	111.34
4	A	264[B]	1CR	NN7-NN8-NN9	-3.17	104.92	107.31
4	A	264[B]	1CR	CN6-CN5-NN7	-3.03	106.83	111.34
3	A	263[A]	0CR	C22-C23-C24	-3.02	112.90	117.64
3	A	263[A]	0CR	C08-C07-C02	3.00	127.75	123.56
4	A	264[B]	1CR	CI5-NN9-CN6	-2.98	122.80	129.82
4	A	264[B]	1CR	C22-C42-C37	2.98	127.73	123.56
4	A	264[B]	1CR	C15-C16-C21	2.95	127.68	123.56
4	A	264[B]	1CR	O08-C52-C60	2.94	118.68	108.72
3	A	263[A]	0CR	C22-C23-C28	2.87	127.57	123.56
3	A	263[A]	0CR	C29-C30-C31	-2.85	113.17	117.64
4	A	264[B]	1CR	C46-O04-C11	2.80	121.76	117.53
3	A	263[A]	0CR	C29-C30-C35	2.75	127.41	123.56
3	A	263[A]	0CR	O04-C11-C12	2.74	121.40	115.73
4	A	264[B]	1CR	C21-C01-C02	2.74	118.61	112.91
3	A	263[A]	0CR	C15-C16-C21	2.68	127.31	123.56
3	A	263[A]	0CR	C66-C67-C61	2.68	122.22	119.45
4	A	264[B]	1CR	C66-C67-C61	2.68	122.22	119.45
4	A	264[B]	1CR	O52-CO5-CI6	2.67	122.62	114.03
4	A	264[B]	1CR	C22-C42-C41	-2.66	113.46	117.64
4	A	264[B]	1CR	O06-C39-C40	2.63	121.17	115.73
3	A	263[A]	0CR	C36-C35-C30	2.61	127.21	123.56
4	A	264[B]	1CR	O04-C11-C12	2.55	118.97	115.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	264[B]	1CR	C29-C30-C35	2.55	127.12	123.56
4	A	264[B]	1CR	O06-C47-C51	2.51	117.21	108.72
4	A	264[B]	1CR	C08-C07-C02	2.51	127.07	123.56
4	A	264[B]	1CR	C51-O05-C12	-2.47	111.63	117.69
3	A	263[A]	0CR	C62-C61-S1	-2.46	116.17	119.73
4	A	264[B]	1CR	C62-C61-S1	-2.46	116.17	119.73
3	A	263[A]	0CR	C10-C11-C12	-2.45	116.58	119.84
3	A	263[A]	0CR	O14-S1-C61	2.38	110.00	107.35
4	A	264[B]	1CR	O14-S1-C61	2.38	110.00	107.35
3	A	263[A]	0CR	O01-C04-C03	-2.34	118.20	123.58
4	A	264[B]	1CR	C26-C27-C28	2.34	124.83	121.09
4	A	264[B]	1CR	C70-C71-C72	-2.24	124.21	128.45
4	A	264[B]	1CR	C15-C16-C17	-2.23	114.14	117.64
4	A	264[B]	1CR	C10-C11-C12	-2.22	116.89	119.84
3	A	263[A]	0CR	C27-C28-C23	-2.19	115.98	118.85
3	A	263[A]	0CR	C26-C27-C28	2.18	124.57	121.09
4	A	264[B]	1CR	C22-C23-C24	-2.17	114.24	117.64
3	A	263[A]	0CR	C22-C42-C41	-2.16	114.24	117.64
4	A	264[B]	1CR	CN4-NN6-NN5	-2.16	105.12	109.45
3	A	263[A]	0CR	C12-C13-C14	2.14	124.51	121.09
3	A	263[A]	0CR	C20-C19-C18	-2.14	117.00	119.84
4	A	264[B]	1CR	C15-C14-C09	2.05	126.43	123.56
3	A	263[A]	0CR	C19-C20-C21	2.04	124.36	121.09
4	A	264[B]	1CR	C27-C28-C23	-2.03	116.19	118.85
3	A	263[A]	0CR	C15-C14-C13	-2.02	114.47	117.64
3	A	263[A]	0CR	CI3-NN6-CN4	-2.01	125.10	129.82

There are no chirality outliers.

All (90) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	263[A]	0CR	C68-C69-N4-N3
3	A	263[A]	0CR	NN6-CI3-CI4-CO3
4	A	264[B]	1CR	C71-C70-O10-C26
4	A	264[B]	1CR	CI6-CI5-NN9-CN6
4	A	264[B]	1CR	NN6-CI3-CI4-CO3
3	A	263[A]	0CR	C13-C12-O05-CT5
3	A	263[A]	0CR	C11-C12-O05-CT5
3	A	263[A]	0CR	C52-C60-O04-C11
3	A	263[A]	0CR	C20-C19-O08-CT3
4	A	264[B]	1CR	C27-C26-O10-C70
4	A	264[B]	1CR	C25-C26-O10-C70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	263[A]	0CR	C18-C19-O08-CT3
3	A	263[A]	0CR	C26-C25-O09-C56
4	A	264[B]	1CR	C51-C47-O06-C39
4	A	264[B]	1CR	O06-C47-C51-O05
3	A	263[A]	0CR	C24-C25-O09-C56
3	A	263[A]	0CR	C38-C39-O06-C59
4	A	264[B]	1CR	C17-C18-O07-C59
4	A	264[B]	1CR	C10-C11-O04-C46
4	A	264[B]	1CR	O08-C52-C60-O09
3	A	263[A]	0CR	O11-C46-C47-O01
3	A	263[A]	0CR	CN3-CT3-O08-C19
3	A	263[A]	0CR	C40-C39-O06-C59
4	A	264[B]	1CR	C19-C18-O07-C59
4	A	264[B]	1CR	C40-C39-O06-C47
4	A	264[B]	1CR	C12-C11-O04-C46
4	A	264[B]	1CR	C38-C39-O06-C47
3	A	263[A]	0CR	CN5-CT5-O05-C12
3	A	263[A]	0CR	C33-C32-O03-C51
3	A	263[A]	0CR	C39-C40-O12-C52
3	A	263[A]	0CR	C64-C65-C68-C69
4	A	264[B]	1CR	C11-C12-O05-C51
3	A	263[A]	0CR	C66-C65-C68-C69
3	A	263[A]	0CR	C12-C11-O04-C60
4	A	264[B]	1CR	CI3-CI4-CO3-O31
4	A	264[B]	1CR	CI3-CI4-CO3-O32
4	A	264[B]	1CR	C24-C25-O09-C60
4	A	264[B]	1CR	C32-C33-O11-CT5
4	A	264[B]	1CR	C33-C32-O03-C56
4	A	264[B]	1CR	C26-C25-O09-C60
4	A	264[B]	1CR	C39-C40-O12-CT3
4	A	264[B]	1CR	C13-C12-O05-C51
3	A	263[A]	0CR	C71-C58-O02-C05
3	A	263[A]	0CR	C17-C18-O07-C57
3	A	263[A]	0CR	C31-C32-O03-C51
3	A	263[A]	0CR	C46-C47-O01-C04
3	A	263[A]	0CR	C27-C26-O10-C70
4	A	264[B]	1CR	C58-C56-O03-C32
4	A	264[B]	1CR	C68-C69-N4-C72
4	A	264[B]	1CR	CI4-CI3-NN6-CN4
3	A	263[A]	0CR	O07-C57-C70-O10
3	A	263[A]	0CR	C41-C40-O12-C52
3	A	263[A]	0CR	NN9-CI5-CI6-CO5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	263[A]	0CR	CI3-CI4-CO3-O31
3	A	263[A]	0CR	CI3-CI4-CO3-O32
3	A	263[A]	0CR	C19-C18-O07-C57
3	A	263[A]	0CR	C06-C05-O02-C58
4	A	264[B]	1CR	C04-C05-O02-C58
3	A	263[A]	0CR	CI5-CI6-CO5-O51
4	A	264[B]	1CR	C52-C60-O09-C25
3	A	263[A]	0CR	C10-C11-O04-C60
4	A	264[B]	1CR	C20-C19-O08-C52
3	A	263[A]	0CR	C05-C04-O01-C47
3	A	263[A]	0CR	C47-C46-O11-C33
3	A	263[A]	0CR	C34-C33-O11-C46
3	A	263[A]	0CR	CI5-CI6-CO5-O52
4	A	264[B]	1CR	C41-C40-O12-CT3
4	A	264[B]	1CR	C31-C32-O03-C56
3	A	263[A]	0CR	C65-C68-C69-N4
4	A	264[B]	1CR	C65-C68-C69-N4
4	A	264[B]	1CR	C34-C33-O11-CT5
4	A	264[B]	1CR	C56-C58-O02-C05
3	A	263[A]	0CR	C70-C57-O07-C18
3	A	263[A]	0CR	C04-C05-O02-C58
3	A	263[A]	0CR	C25-C26-O10-C70
4	A	264[B]	1CR	CI6-CI5-NN9-NN8
3	A	263[A]	0CR	C68-C69-N4-C72
3	A	263[A]	0CR	C32-C33-O11-C46
4	A	264[B]	1CR	CN3-CT3-O12-C40
4	A	264[B]	1CR	C06-C05-O02-C58
4	A	264[B]	1CR	C18-C19-O08-C52
3	A	263[A]	0CR	O12-C52-C60-O04
4	A	264[B]	1CR	O03-C56-C58-O02
4	A	264[B]	1CR	C60-C52-O08-C19
3	A	263[A]	0CR	C62-C61-S1-O13
3	A	263[A]	0CR	C67-C61-S1-O13
4	A	264[B]	1CR	C62-C61-S1-O13
4	A	264[B]	1CR	C67-C61-S1-O13
3	A	263[A]	0CR	C03-C04-O01-C47
3	A	263[A]	0CR	CI6-CI5-NN9-CN6

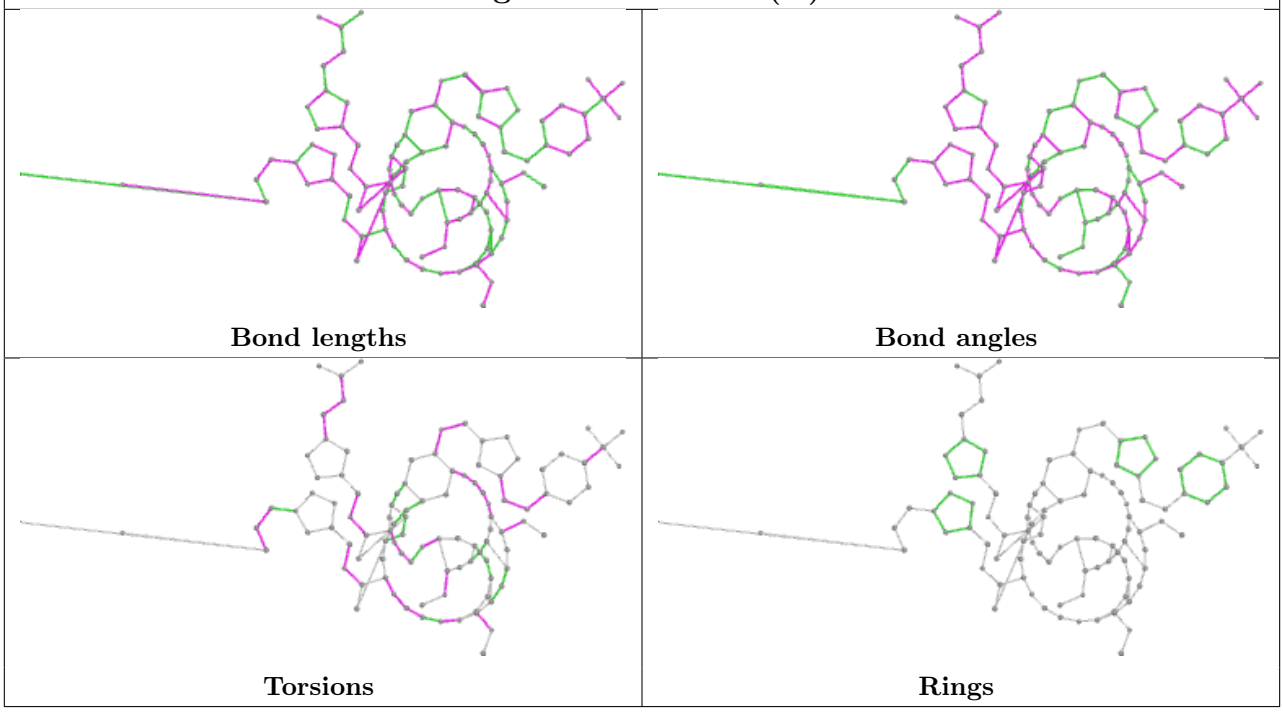
There are no ring outliers.

2 monomers are involved in 11 short contacts:

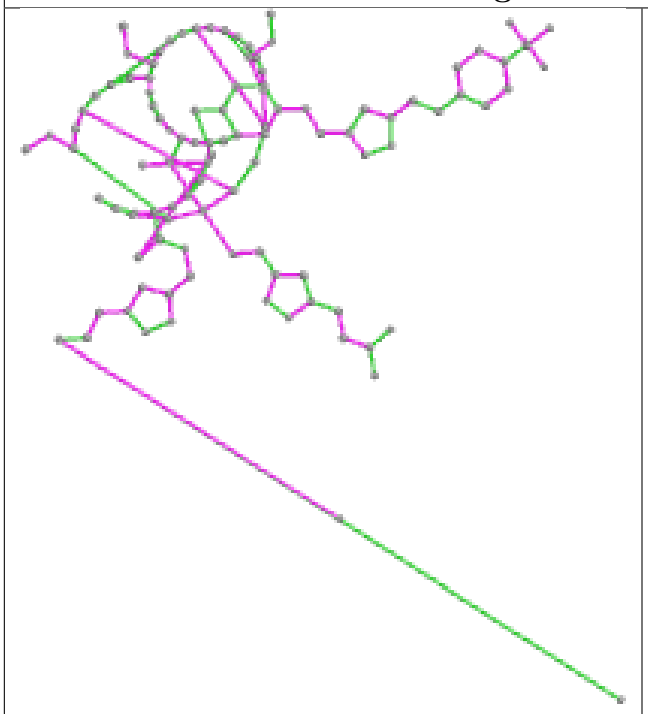
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	263[A]	0CR	4	0
4	A	264[B]	1CR	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

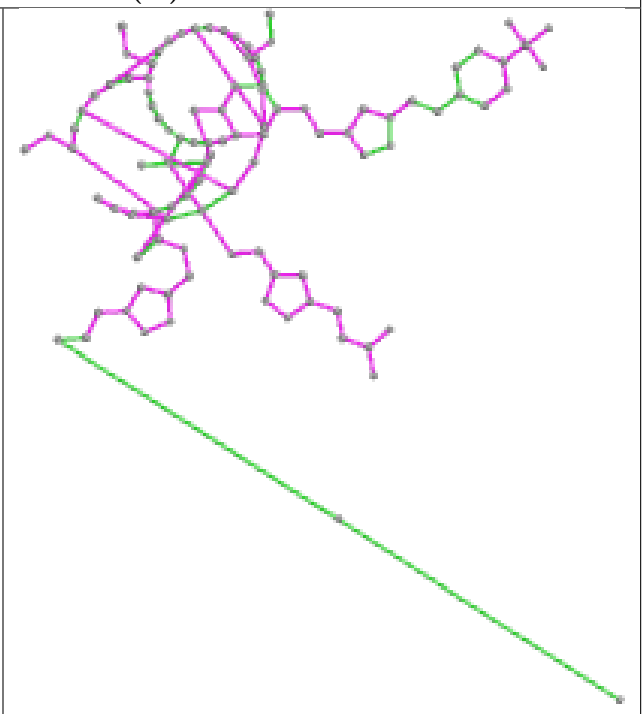
Ligand 0CR A 263 (A)



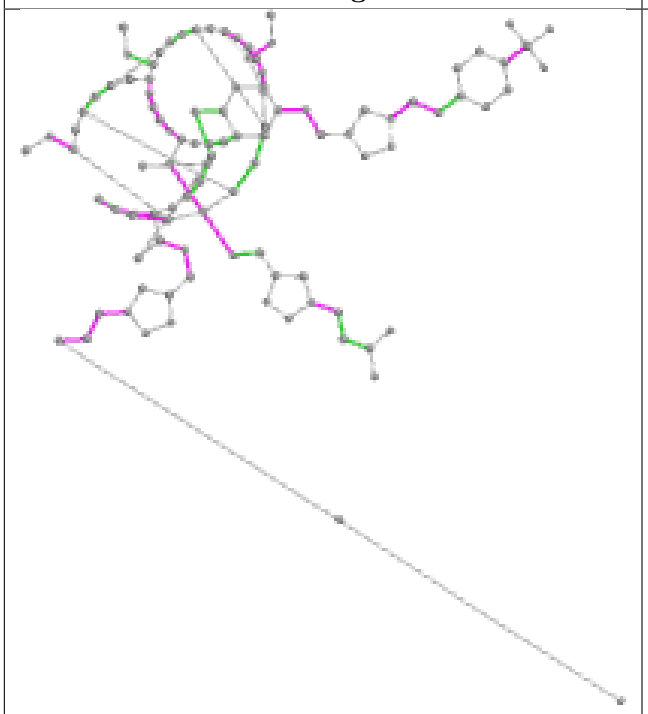
Ligand 1CR A 264 (B)



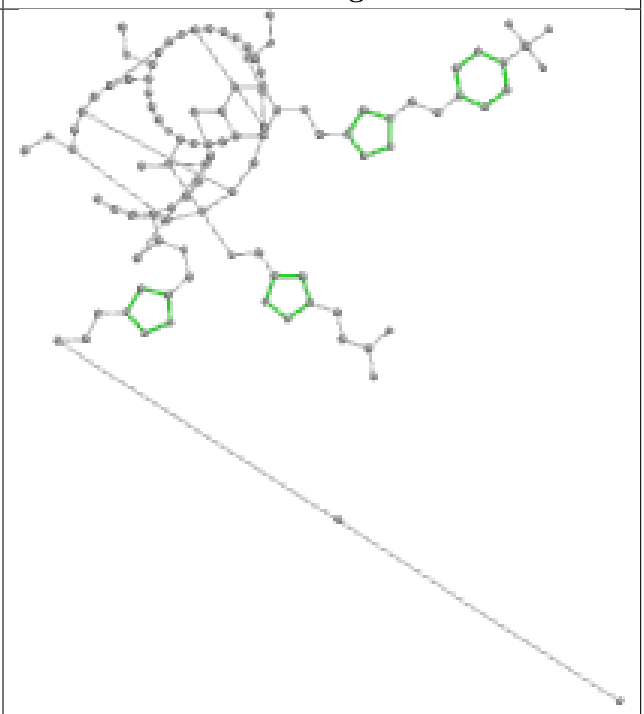
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	257/260 (98%)	-0.17	5 (1%) 66 70	21, 31, 45, 62	2 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	76	LYS	3.4
1	A	235	GLY	3.3
1	A	4	HIS	2.9
1	A	237	PRO	2.6
1	A	261	LYS	2.4

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	0CR	A	263[A]	103/103	0.60	0.57	29,42,44,45	103
4	1CR	A	264[B]	103/103	0.65	0.56	29,44,47,47	103

Continued on next page...

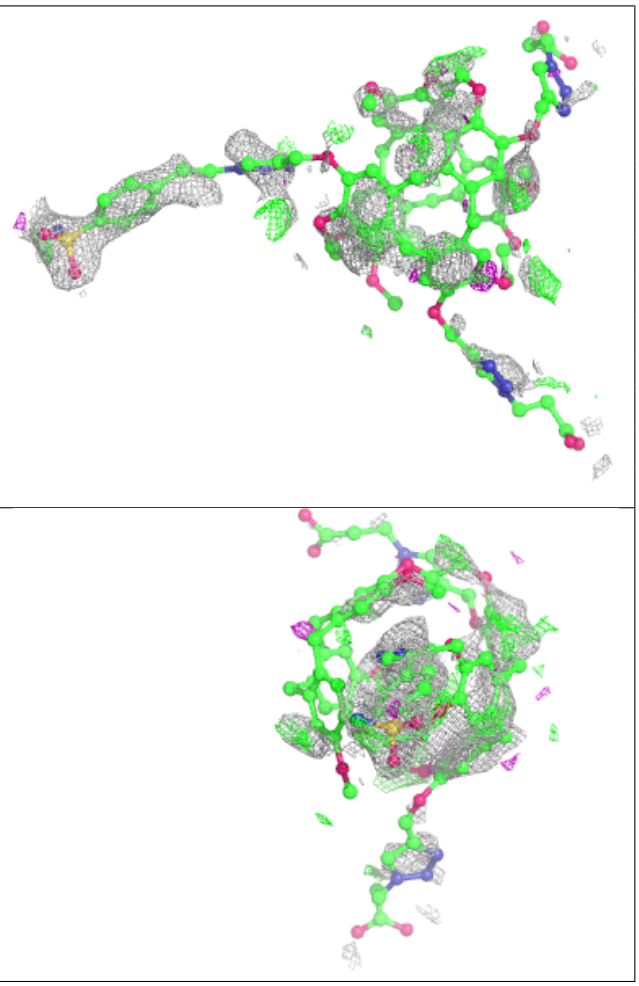
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	XE	A	266	1/1	0.91	0.07	42,42,42,42	1
5	XE	A	265	1/1	0.98	0.08	44,44,44,44	1
2	ZN	A	262	1/1	0.98	0.07	27,27,27,27	1

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

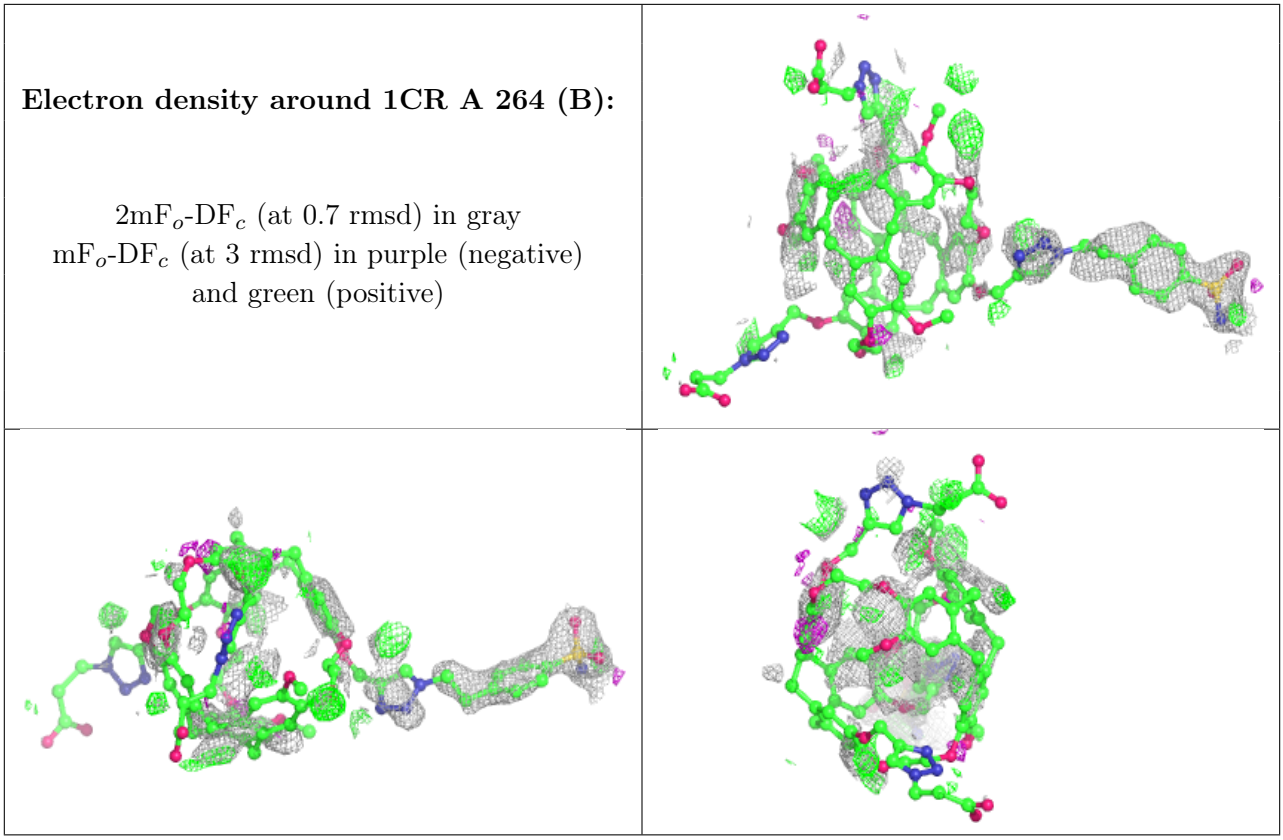
Electron density around 0CR A 263 (A):

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 1CR A 264 (B):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.